2014

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Environmental Modelling & Software xxx (2014) 1–12

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

A decision making framework with MODFLOW-FMP2 via optimization: Determining trade-offs in crop selection☆

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ARTICLE INFO

Article history:
Received 16 April 2014
Received in revised form
19 November 2014
Accepted 24 November 2014
Available online xxx

Keywords:
Simulation-based optimization
Multi-objective
Farm management

ABSTRACT

Farmers in regions experiencing water stress or drought conditions can struggle to balance their crop portfolios. Periods of low precipitation often lead to increased, unsustainable reliance on groundwater-supplied irrigation. As a result, regional water management agencies place limits on the amount of water which can be obtained from groundwater, requiring farmers to reduce acreage for more water-intensive crops or remove them from the portfolio entirely. Real-time decisions must be made by the farmer to ensure viability of their farming operation and reduce the impacts associated with limited water resources. Evolutionary algorithms, coupled with accurate, flexible, realistic simulation tools, are ideal mechanisms to allow farmers to assess scenarios with regard to multiple, competing objectives. In order to effective, however, one must be able to select among a variety of simulation tools and optimization algorithms. Many simulation tools allow no access to the source code, and many optimization algorithms are now packaged as part of a suite of tools available to a user. In this work, we describe a framework for integrating these different software components using only their associated input and output streams. We analyze our strategy by coupling a multi-objective genetic algorithm available in the DAKOTA optimization suite (developed and distributed by Sandia National Laboratory) with the MODFLOW-FMP2 simulation tool (developed and distributed by the United States Geological Survey). MODFLOW-FMP2 has been used extensively to model hydrological and farming processes in agriculture-dominated regions, allowing us to represent both farming and conservation interests. We evaluate our integration by considering a case study related to planting decisions facing farmers experiencing water stress. We present numerical results for three competing objectives associated with stakeholders in a given region (i.e., profitability, meeting demand targets, and water conservation). The data obtained from the optimization are robust with respect to algorithmic parameter choices, validating the ability of the associated evolutionary algorithm to perform well without expert guidance. This is integral to our approach, as a motivation for this work is providing decision-making tools. In addition, the results from this study demonstrate that output from the chosen evolutionary algorithm provides a suite of feasible planting scenarios, giving farmers and policy makers the ability to compromise solutions based on realistic simulation data.

1. Introduction

Recent water crises in the agriculture-intensive states of California and Kansas highlight the difficulties associated with managing limited resources in the context of various competing interests. California water management agencies have dealt with consequences of drought for many years. In fact, a 2011 report by the Public Policy Institute of California (PPIC) (Hanak et al., 2011)

☆ Thematic Issue on the Evolutionary Algorithms.

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http://dx.doi.org/10.1016/j.envsoft.2014.11.031
1364-8152/

recognized the need for improved water management practices. In 2014, many aquifers are still pumped at an unsustainable level (Chappelle et al., 2014) and, until recently, local water management agencies lacked the authority to develop and implement water management plans (Chappelle et al., 2014). While California as a whole has become less dependent on agriculture for its economic success (Chappelle et al., 2014), farmers still consume a majority of the groundwater resources available in the state (Hanak et al., 2011; Kenny et al., 2009; Maupin et al., 2014). Thus, water policy decisions have a larger impact on farmers than on other users of groundwater, and changes in farming practices have a significant impact on the overall availability of the groundwater resources.

Part of the motivation for this work is the vital need to assess the impact of farming practices on groundwater resources and to evaluate different scenarios of a farm model to guide decision makers. The use of mathematical modeling and optimization in planning crop strategies is well-documented (see, for instance, Dury et al., 2011 and references therein El Nazer and McCarl, 1986; Baker and McCarl, 1982; Beneke and Winterboer, 1984; Sahoo et al., 2006; Annetts and Audsley, 2002; Lehmann et al., 2013; Groot et al., 2012). In addition, the application of optimization methods (specifically evolutionary algorithms, described in detail below) to real-world problems to guide decision making has been identified as a key research challenge (Maier et al., 2014). In particular, the study here is aligned with trying to understand the algorithm performance across a set of algorithm parameters with no corresponding analytic solution for comparison as the underlying problem requires a simulation incorporating real data. In addition, we identify challenges associated with this approach to point the way towards future work. This study is therefore directly aligned with current research challenges and future directions (Maier et al., 2014) with regards to “the mathematical formulation of objectives and constraints for real world problems” as well as “the development and understanding of limitations and strategies for increasing relevance and credibility.”

Any modeling and optimization strategy intending to aid farmers in decision making must be able to account for multiple, competing objectives. For example, attempting to maximize profit may require growing more water intensive crops. In regions experiencing drought, simultaneously minimizing water usage is critical but can be in conflict with the profit objective. In addition, the farming process itself is dynamic, with farmers naturally transitioning farm states based on previous crop performances and availability of resources. The performance of the crop portfolio depends, in part, on the availability of water, the nutrients available in the soil (which may depend on previous plot allocations), and the water requirements of the crops. In order to meet irrigation requirements for the crops, farmers often incorporate a variety of irrigation methods, including pumping and surface water delivery systems (Schmid and Hanson, 2009). The mechanism for water delivery determines the efficiency of the farm; the health of supply aquifers determines any extraction limits on the pumping wells. There is no single planting schedule that will simultaneously satisfy all the stakeholders it will impact; in fact, individual farmers in a given region with the same base crop portfolio may make different planting decisions based solely on personal goals.

Groundwater resources have become critically strained, as overuse, in conjunction with extreme droughts, has placed aquifers in jeopardy of overdraft. Nearly 70% of groundwater withdrawals are used for irrigation, and nearly 90% of the groundwater used for agricultural irrigation is drawn from 13 states (Kenny et al., 2009; Maupin et al., 2014). Groundwater is the primary source of irrigation in Nebraska, Arkansas, Texas, Kansas, Mississippi, and Missouri (Kenny et al., 2009; Maupin et al., 2014). Portions of several of these states (Nebraska, Kansas, and Texas) overlay parts of the High Plains Aquifer, located in the Midwest region of the United States. Previous studies on the High Plains Aquifer have considered different water management strategies (McGuire et al., 2002; Peterson and Ding, 2004; Scanlon et al., 2012; Musick et al., 1990; Sophocleous, 2010), and stories of possible depletion of the High Plains Aquifer have headlined recent news programs (Morris, 2013; Charles, 2013). Farmers in these regions have agreed to reduce their irrigation, but long-term impacts on available water resources and profitability of the associated farms remains largely unknown.

Details of the underlying hydrological system, water delivery systems, climate information, and plant attributes are essential to guiding model-based planting decisions. To this end, it is necessary to use a simulation tool that incorporates these aspects of the farming cycle. Moreover, an approach that is scalable from a single farm to an agricultural region, including multiple farms and large-scale hydrological and geological attributes, can guide both individual farmers and policy makers. Several packages for farm simulation exist (Keating et al., 2003; Stöckle et al.; Groot et al., 2012), each focusing on different aspects of the plant–soil interactions. Specifically, these approaches model individual farms with mechanisms for simulating crop rotation, irrigation, fertilization, and plant growth dynamics. These simulation-tools have successfully been paired with optimization algorithms to improve farm management (Groot et al., 2012; Klein et al., 2012; Lehmann et al., 2013; Sommer et al., 2010).

Recent efforts in understanding water resources have sought to incorporate details on agricultural impact, both on a macro-scale and an individual farm scale (Schmid and Hanson, 2007, 2009; Condon and Maxwell, 2014a, 2014b). MODFLOW was developed originally by the United States Geological Survey (USGS) in the 1980's to model groundwater flow in confined and unconfined aquifers. Its basic functionality has grown significantly over the years and has been extended for use in agricultural applications through the USGS Farm Process (FMP2) (Schmid and Hanson, 2009; Hanson et al., 2014a). FMP2 was developed in collaboration with the Pajaro Valley (California) Water Management Agency (PVWMA) to better simulate irrigated agricultural systems and hence accurately forecast supply-and-demand scenarios to help policy makers (Schmid and Hanson, 2007, 2009). This ability to study the often competing interests of farmers, residential users, and environmental agencies is critical to assess the impacts of water withdrawals from a variety of sources in the context of potential climate uncertainty (Hanson et al., 2012).

The utility of the MODFLOW-FMP2 software has been demonstrated on many application areas, including the Pajaro, Central, and Cuyama Valleys in California (Faunt, 2009; Hanson et al., 2010, 2014b, 2014c; Hanson and Sweetkind, 2014), the Lower-Rio Grande region in Texas (Hanson et al., 2013), and the Southern Rincon Valley in New Mexico (Schmid and King, 2009). In addition, the MODFLOW-FMP2 framework can be used to study conjunctive use agricultural models (Hanson et al., 2010; Hanson and Schmid, 2013; Schmid and King, 2009), allowing for irrigation strategies using surface-water or groundwater. The ability of MODFLOW-FMP2 to model multiple components of the water cycle, including incorporation of precipitation events, has also allowed its use in the study of aquifer recharge and other basin management systems (Hanson et al., 2008, 2014c; Hanson and Lockwood, 2012; Schmidt et al., 2012).

Despite the numerous case studies involving the MODFLOW-FMP2 simulation tool, it has yet to be used in a decision making framework utilizing optimization algorithms to seek optimal strategies for water management. Facilitating the use of MODFLOW-FMP2 with independently-developed optimization software provides a powerful new tool for decision makers. MODFLOW-FMP2 as a simulator has already been used to influence policy and planning

(Hanson et al., 2013, 2014b). However, its use within a flexible optimization framework where model inputs can instead become decision variables and model outputs can be used in mathematical representations of resource management goals has not yet been tested. This framework provides a tool in which stakeholders can define their own objectives and still benefit from the sophisticated modeling capabilities of the simulator.

Our focus in this work is the applicability of evolutionary algorithms (EAs) to aid in agricultural decision making in terms of crop selection using MODFLOW-FMP2 output. Evolutionary algorithms are a member of the class of metaheuristic algorithms whose candidate solutions to the optimization problem are chosen based on evolutionary principles, for example mutation, reproduction, and survival of the fittest (Holland, 1992; Maier et al., 2014). EAs are part of a broader class of optimization methods called derivative-free or sampling algorithms because the search for optimality is guided only by function evaluations. Classical methods for optimization require locating critical points by setting the gradient of the objective function to zero. For simulation-based optimization problems, gradients may be difficult or impossible to determine and approximations may be unreliable due to low-amplitude noise from the simulation output. Thus, sampling methods such as an EA are suitable for non-differentiable, non-convex, and discontinuous objective functions. The use of EAs for a simulation-based crop-planning first appeared in 2006 (deVoil et al., 2006). The authors recognized the need for farming decisions to balance competing objectives, requiring robust models as a tool to support the decision-making process. More recent work pairing EAs with simulation tools focuses on plant–soil interaction modeling with an emphasis on bio-economic models in the presence of climate change or policy constraints (Lehmann et al., 2013; Groot et al., 2012; Lautenbach et al., 2013; deVoil et al., 2006). These studies imply that the suite of feasible scenarios generated by an EA can lead to significant improvement in farm-management in the presence of competing objectives when compared to only evaluating the model itself at a set of selected planting options. However, none of the studies focused on dynamic water allocations needed for irrigation strategies using a regional scale hydrological and agricultural model.

Towards this end, we used datasets for crops and subsurface models included in the FMP2 download as tests cases for our study. These datasets were generated using realistic parameter values for typical crops and aquifers found in California; building our own datasets would have incorporated uncertainty with regards to the feasibility of our data into our study. We chose crops across the spectrum of profitability and water usage to ensure competition between potential objectives of different stakeholders.

In fact, the multiple competing objectives functions presented in this study were developed by working together with farmers from Reitter Affiliated Companies (http://www.berry.net/) in an initial attempt to address concerns about water usage in the Pajaro Valley berry growing region. Preliminary results from an optimization study that did not use an underlying simulation tool have already led to changes in farming practices (Bokhiria et al., 2014; Kupec, 2014). The ability to represent the farming cycle's impact on water resources and the environment will further advance sustainable farming practices. Collaborations between mathematicians, environmental engineers, farmers, and policy makers are necessary and the hope is this decision support tool can aid in that process. This need is clearly stated in the Position Paper from this Thematic Issue (Maier et al., 2014) and we attempt here to demonstrate how optimization can be applied to consider management alternatives using a reliable and powerful underlying model.

We proceed by describing the multi-objective models used for decision making in Section 2 and the simulation and optimization software in Section 3. Numerical experiments and a discussion of the results, including optimization landscapes, are in Section 4 and discussion and future research directions are in Section 5.

2. Problem formulation

The overarching optimization approach requires objective functions to represent a farmers goals. These objectives may include consideration of revenue and available resources. Ultimately the farmer must choose which crops to plant to satisfy those personal objectives. Given a set of N_C crops, we choose as decision variables the percentages of each crop planted at the time a decision is made. Decision points occur over a growing season as crops are harvested, making previously occupied land available. Farmers must opt to plant another crop or allow the land to "rest". Each crop in the portfolio has its own planting schedule, meaning it may be planted one or more times per year. In those cases where a crop can be planted more than once per year (e.g., lettuce, which can be planted every four months in some regions of the country), a decision variable is required at each planting opportunity. The choice to plant based on the growing season means including a decision variable only at the time of a planting opportunity, allowing the optimization algorithm to act as a virtual farmer. We let x_i^k denote the percentage total acreage allocated to crop i planted at the kth opportunity. We remove the superscript if there is one planting opportunity for the crop.

In addition, various stakeholders in a given region may have competing interests resulting in different planting schemes. Stakeholders in a region may include farmers, nonagricultural landowners, ranchers, industries, developers, and residents. For instance, farmers in a region would like to maintain profitability, but must operate under water use restrictions imposed by water management agencies. Crops differ in the amount of water required, and farmers must make decisions when more profitable crops require more water. Imbalances between supply and demand, in large part, determine the profitability of a given crop. During periods of limited water availability, crops with higher water usage have reduced supply, potentially increasing their profitability.

Integral to our study is a desire for flexibility so that the simulation-based framework can easily be used for various performance metrics, depending on the stakeholders being considered. We consider three objectives to demonstrate the capability of the framework. Note, however, one of the advantages of simulation-based optimization is the ability to define objective functions outside the simulation tool; that is, the objective functions rely only on output from the simulation model. Thus, any modeling input or output could be adapted as a decision variable or used within objective function and constraint evaluations, respectively.

For this work, we consider growing practices that can maintain profitability while also minimizing pumping to ensure sustainable aquifer utilization. Additionally we know that in reality there exists pressure due to market demands for crops of a certain type, which if unmet can strongly change a grower's business dynamic. All three of these objectives are naturally competing with almost exclusively a low pumping crop option also being less profitable, a high profit crop being a high water usage crop and demand being driven by (often unpredictable) trends in consumer tastes/preferences at the time of planting. We describe the three objectives in our formulation and necessary constraints below.

2.1. Objective functions

The underlying purpose of the optimization problem is to select crops based on trade-offs between revenue, water-use, and demand objectives. These objectives aim to provide a farmer with a suite of feasible farm states that allow for crop selection based on individual farming goals. We consider the simplified case associated with one planting decision for each crop (i.e. x_i, $i = 1,\ldots,N_c$) and then those crops grow, yield, and are replanted with the same distribution over two years. We chose to have one planting decision made over a two year time frame not only to facilitate the problem formulation, but also because conversations with berry farmers in the Pajaro Valley of California indicated that, as a rule of thumb, they will not significantly modify crop planting decisions by more than 20% from year to year. In addition, the water and sales prices, provided by the farmers and presented in (Bokhiria et al., 2014), show there are time frames over which those values do not vary significantly. The design space in this case is easier to analyze than the case that involves changing the crop distribution after a harvest. This allows us to focus more attention on the performance of the optimizer relative to the performance of the simulator and the evaluations of the objective functions.

We calculate the revenue generated from a crop portfolio as the sales price times the yield of each crop minus the cost of water required for irrigation. This is given by

$$\text{Maximize } P = \sum_{i=0}^{N_c} [x_i \times Y_i \times C_i \times A] - C_w \times W_{gw}, \tag{1}$$

where the decision variable x_i is the fraction of crop i, Y_i is the total yield for crop i (Weight/L^2), C_i is the sales price of crop i ($/Weight), A is the acreage of the farm, C_w is the cost of groundwater pumping ($/$L^3$), and W_{gw} is the volume of water extracted from the aquifer (L^3). Alternative revenue models could incorporate seed and labor costs for the distribution of different crops as well as time varying water prices (Bokhiria et al., 2014).

Water usage is based on the volume of water obtained per day (units L^3/T) via groundwater extraction. Let N_{wells} denote the number of pumping wells in the model. The second objective is given by

$$\text{Minimize } W_{gw} = \sum_{t=0}^{t_f} \sum_{j=1}^{N_{wells}} V_{tj}, \tag{2}$$

where V_{tj} is the volume of water extracted from well j at time step t, and t_f is the final time for extraction. Given an initial farm state, the MODFLOW-FMP2 simulation tool provides a volume of water obtained from groundwater pumping at each time step. In addition, the user is allowed to limit the total amount of pumping; we chose 13,000 m^3/day as a pumping limit.

For the last objective, we seek to minimize the l_2 norm of the deviation from a specified demand

$$\text{Minimize } D = \|Y_a - Y_d\|_2 = \sqrt{\sum_{i=1}^{N_c} (Y_a)_i - (Y_d)_i}, \tag{3}$$

where $(Y_a)_i$ is the actual yield (Weight) and $(Y_d)_i$ is the demand yield (Weight) for crop i. For any crop, the yield, Y_a, is not calculated by MODFLOW-FMP2 but can be approximated based on the evapotranspiration data provided as output by the simulator. We use a model given by the Food and Agriculture Organization of the United Nations (FAO) (Steduto et al., 2012).

$$\left(1 - \frac{Y_a}{Y_m}\right) = K_y\left(1 - \frac{ET_a}{ET_m}\right), \tag{4}$$

where Y_m is the maximum yield in unstressed conditions (Weight), ET_a is the actual crop evapotranspiration (L/T), K_y is the crop water production response coefficient, and ET_m is the maximum crop evapotranspiration in unstressed conditions (L/T).

We can find the maximum crop evapotranspiration ET_a given a known reference evapotranspiration (ET_0) and crop coefficient (K_c) using

$$ET_m = ET_0 \times K_c.$$

In practice, given a reasonable estimate on the unstressed yield for a given crop and the actual crop evapotranspiration, we can estimate the actual yield for a given crop in both stressed and unstressed conditions, extending the robustness of our results to account for drought scenarios.

Since our decision variables are the fraction of each type of crop, we require

$$\sum_{i=1}^{N_c} x_i \le 1 \tag{5}$$

at each planting decision. Note this also allows land to go fallow.

3. Simulation-based optimization software

One of the main deliverables of this work is providing a framework facilitating the linkage between MODFLOW-FMP2 and an optimization algorithm. For optimization, we use DAKOTA, a software package from Sandia National Labs (Adams et al., 2009). However, one of the primary purposes of this study was to understand the applicability of MODFLOW-FMP2 within a flexible simulation-based setting, so ultimately any derivative-free optimizer could be used. We proceed by describing this process and provide background on the multi-objective genetic algorithm used in the DAKOTA framework.

3.1. Wrapper design

Performance-based analysis of simulation-based optimization is challenging, in part, because one must construct a flexible software coupling between an optimizer and the simulation tools. The coupling framework must obtain values of decision variables from the optimization algorithm, construct input files for the simulation tool, run the associated simulation, and return to the optimizer the data needed for evaluation of the objective functions and constraints. It is straightforward, although potentially tedious, to write the necessary computational instructions for one coupling of one optimization algorithm and one simulation tool. The task is more complicated if one wishes to analyze the performance of multiple algorithms over a suite of simulation tools and problem formulations.

We developed a communication tool between DAKOTA and MODFLOW-FMP2 using object-oriented design to abstract both the MODFLOW-FMP2 simulation and the optimization problem into easily managed classes. We chose Python to implement the abstraction, but the concepts can be realized in any language with reasonable object-oriented support. This simplifies the process of defining realistic farm systems, allowing us to focus on important features of the system, instead of manipulating input files. Fig. 1 contains a flow chart showing the extent to which we are abstracting the individual model components and the cyclic flow of information throughout the optimization process.

Crop and farm properties are defined as instances of their respective classes using a script. The object-oriented design enables modifications of the input parameters in a simulation as well as direct manipulations of any simulation parameter. Complete descriptions of the input requirements for MODFLOW-FMP2 and

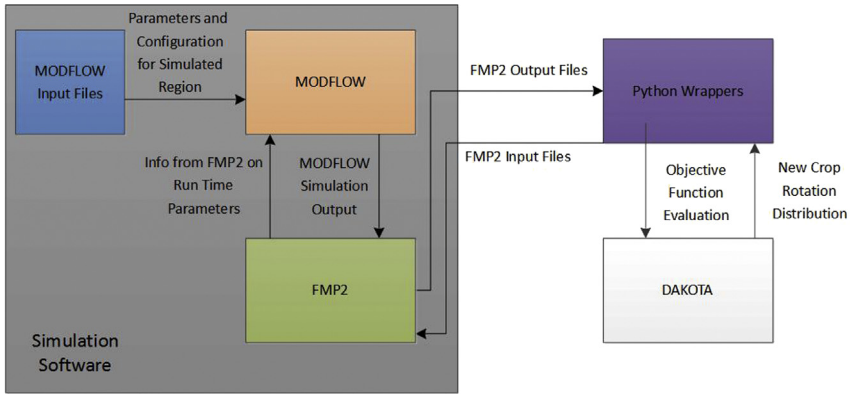


Fig. 1. Framework for pairing MODFLOW-FMP2 with DAKOTA. The user can provide any objective functions of interest using output from the simulation tool and use any input to FMP2 as decision variables.

MODFLOW are provided in their respective user's manuals (Schmid and Hanson, 2009; Harbaugh, 2005). The wrappers used in this work as well as the objective function subroutines and the data files for the test problem described below are available for download at http://people.clarkson.edu/kfowler/Sustainability.html.

3.2. Optimization algorithm

DAKOTA provides a suite of optimization strategies for a range of simulation-based scenarios and is an ideal framework for this study since it is open-source and flexible (Adams et al., 2009). Understanding the applicability of optimization algorithms, in particular evolutionary algorithms, to real-world problems is an active area of research (Maier et al., 2014). As mentioned above, agricultural management requires addressing multiple, competing objectives, and previous studies have shown EAs have performed well in related settings (Lehmann et al., 2013; Groot et al., 2012; Lautenbach et al., 2013; deVoil et al., 2006). To this end, we chose the multi-objective genetic algorithm (MOGA) developed by Eddy and Lewis (2001) and implemented in the DAKOTA framework.

Since the objectives are competing, there is no single solution that simultaneously optimizes each objective. A multi-objective approach instead provides a set of points, giving stakeholders the ability to analyze trade-offs between points. In general, genetic algorithms move through “generations” of evaluation points by assessing the fitness of members of the generation and selecting members to continue to the next generation (through mutation or cloning), parent offspring for the next generation, or die (i.e. removing those points from the population). In a multi-objective setting the population evolves towards a set in which the points are non-dominated, known as a Pareto set. A non-dominated point has the property that its fitness cannot improve with respect to one objective without degrading the value of another.

The basic steps of the algorithm are to initialize a population, evaluate the objective function and constraints, perform crossover and mutation, evaluate the new population members and assess the fitness of each population. Population members are then replaced to continue to the next generation. Termination of the optimization can be based on a maximum number of function evaluations (or iterations) or on performance metrics. The performance metrics track changes in the population from generation to generation. Finally, a post processing step reduces the final solution set so that a minimum distance exists between any two design points. There are a variety of algorithmic parameters that impact the search behavior of MOGAs. The parameter values we considered are specified in Table 1. For this study, we chose to initialize the population randomly and use default settings except that we vary the population size and mutation rate. In particular, we consider four different initial population sizes and two mutation rates to assess their impact on the quality of the solution set. We present those analyses in Section 4.

4. Numerical experiments

The numerical experiments were constructed to evaluate the functionality of the coupling strategy between MODFLOW-FMP2 and an optimization algorithm, the ability of the MOGA to generate feasible solutions, and the sensitivity of our problem formulation. We consider the resulting pumping requirements for selected planting strategies provided by the optimizer to demonstrate the variety of choices provided to farmers. The resulting trade-off curves highlight the nature of the objective functions and the ability of the MOGA to provide a broad range of solutions for the stakeholders. To understand the performance of the MOGA, we considered four different population sizes and two mutation rates and assessed the impact on the final solution sets. In addition, we generate optimization landscapes to gain insight into the design space, which is dependent on the output from MODFLOW-FMP2.

We build our optimization problem using a hydrological model taken from the MODFLOW-FMP2 simulation set, which we describe in detail below. We then describe the crops chosen for this study followed by the results.

4.1. Hydrological setting

The problem formulation used a dataset that was designed to demonstrate the capabilities of MODFLOW-FMP2. We note that while this is a hypothetical test case, the test problems included in the MODFLOW-FMP2 software package are intended to be as realistic as possible (Schmid and Hanson, 2009). Using a representative, pre-validated hydrological model formulation (i.e., using

Table 1
MOGA parameter values (default settings except for population size and mutation rate).

Optimization parameter	Setting	Optimization parameter	Setting
Population sizes	150, 175, 200, 225	Crossover type	Shuffle random
Initialization type	Unique random	Fitness type	Layer rank
Mutation type	Replace uniform	Convergence condition	<5% change over 5 generations
Mutation rates	0.08, 11		

an existing dataset) allows us to focus more attention on the proof-of-concept for the interface and the associated performance of the optimization. The model includes a 10 km by 11.5 km region with multiple farms, urban zones, riparian zones (interfaces between land and streams), and areas of natural vegetation. The water management system includes multiple wells, stream inflows and outflows, and natural precipitation.

The topography slopes downward from west to east and converges from the north and south toward a riparian region along the eastern edge. The underlying geology contains 7 layers: four aquifer layers separated by three layers of confining material (Schmid and Hanson, 2009). The aquifer nearest the surface is unconfined with varying depth. The remaining (confined) layers are uniformly 60 m thick, with each layer of confining material between 5 m and 15 m thick. The saturated hydraulic conductivity (a measure of the ability of the aquifer to transmit fluid) varies from 10 m/d in the aquifer nearest the surface to 0.15 m/d in the aquifer furthest from the surface.

The example region is divided by a stream flowing west to east. The stream flow into the domain is prescribed at 50,000–100,000 cubic meters per day. No fluid flow is allowed into the region through the northern and southern boundaries. The eastern and western boundaries have general head boundaries. These specify a head-dependent flux designed to mimic known groundwater head at a specified distance. The topography and boundary conditions dictate a west-to-east directional groundwater flow.

The model domain consists of a 20×23 grid, where each cell within the grid is associated with a specific farm type. The production farm is modeled using a 10×10 block of cells in the upper left corner of the domain. The riparian vegetation zone is comprised of a block of 25 cells lying along the east boundary, and the remaining cells are associated with native vegetation landscape. A schematic of the model domain is given in Fig. 2, with the different regions represented by distinct colors. The orange cells denote the production farm, the green cells denote the riparian region, and the dark gray cells denote the native vegetation. The blue circles show the locations of the wells, while the blue line represents a stream. The production farm is the focus of the simulation, but the properties associated with the surrounding landscape also affect the dynamics of the simulation.

In practice, the physical composition of the subsurface impacts the optimization as soil properties govern runoff and inefficiencies in the irrigation system. Our test problem consists of three different soil types which are predefined in MODFLOW-FMP2. The soil types are silt, sandy loam, and silty clay. Their distribution is shown in Fig. 3.

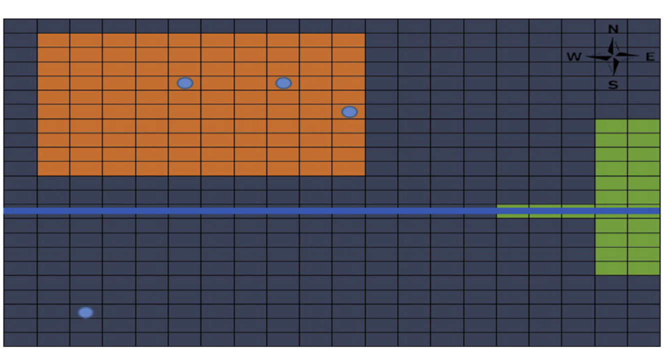


Fig. 2. Diagram of test problem farm configuration. The orange cells denote farm regions, dark gray cells are native vegetation, and green cells are riparian vegetation. The blue line represents a river, and blue circles denote wells. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

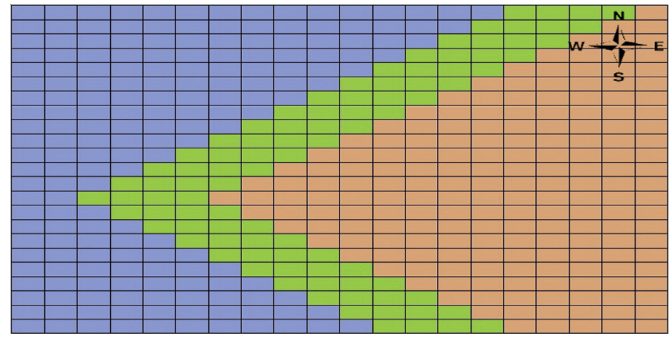


Fig. 3. Distribution of soils throughout our model domain. Light blue cells are silt, green cells are sandy loam and beige cells are silty clay. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Several adjustments were made to allow for a more definitive assessment of the performance of the optimization algorithm and the coupling strategy. In particular, we reduced the number of farms to three; an agricultural farm, a riparian zone, and an area of native vegetation. We consider five crops: three are agricultural products of the farm (our decision variables), one is the vegetation in the riparian zone, and the final is the native vegetation. In this model crops receive water through irrigation or precipitation only, with a uniform distribution across all crops. Four extraction wells are included in the model and all other water delivery options were not used. The crop distribution, which is specified by the optimizer, is set for the entire simulation. We incorporate precipitation data taken from a weather station in California from January 2012–December 2013 (CIMIS, 2014). The volumetric flow rates for the precipitation are shown in Fig. 5 (the dashed line) which varies significantly over the two years and includes two periods of drought.

4.2. Crops

We seek the optimal planting scenario given a system with three options for crop selection based on alfalfa, lettuce, and strawberries, which we refer to as Crop 1, Crop 2, and Crop 3 respectively. Each crop is defined by competing properties. Crop 1 requires the most irrigation, is the most profitable, but has moderate demand. Crop 2 has low irrigation requirements, is the least profitable, and has the lowest demand. Crop 3 uses a moderate amount of irrigation, has moderate profitability, yet has the highest demand of the three crops. Specific model parameters for the crops used in our

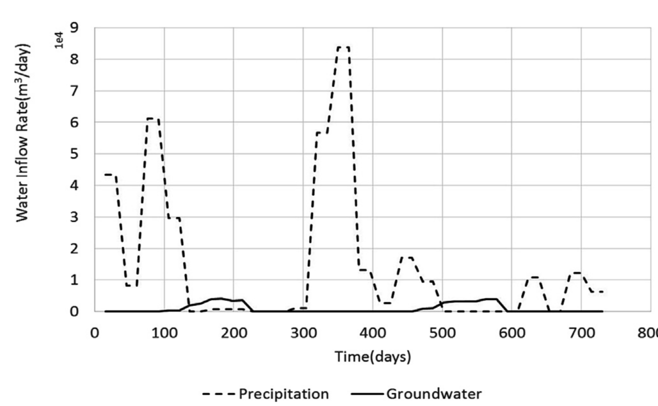


Fig. 4. Water usage from pumping over time (sold line) in relation to the precipitation (dashed line) with crop fractions fixed to those in Table 3.

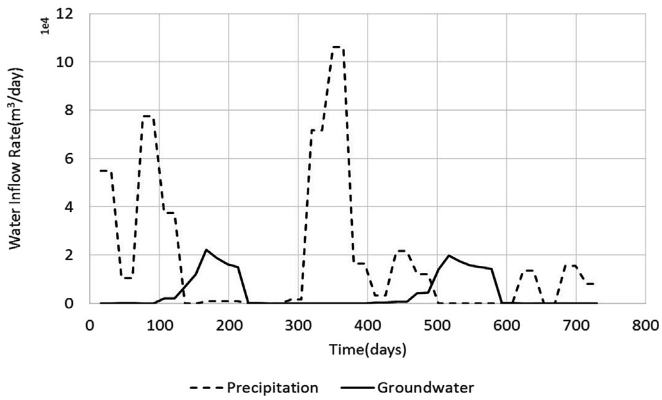


Fig. 5. Water usage from pumping over time (sold line) in relation to the precipitation (dashed line) for crop fractions set to (0.40, 0.12, 0.48).

simulation are provided in a database with the MODFLOW-FMP2 source code.

The objective functions were evaluated using the crop data in Table 2 taken from Undersander (2002), Barnett (2014), Annual Statistics Bulletin (2012), Commodity Pricing, Demchak et al. and Boriss et al. We use $C_w = 0.06$ \$/m^3 as the price of water.

4.3. Results

We performed a suite of numerical experiments using population sizes of 150, 175, 200, and 225 and mutation rates of 0.8 and 0.11. Computations were run on a Linux Workstation with 2× Eight-Core AMD Opteron processors using DAKOTA version 5.4 and MODFLOW-2005 version 1.6.01 with FMP2 compiled using standard optimization flags. Since the MOGA uses random initial populations, optimization trials were run 30 times for each configuration, resulting in a total of 240 optimization runs.

The MOGA offers a final set of solutions so that stakeholders can observe trade-offs and analyze design points to aid in planting choices. Recall with competing objectives there is no single solution that will optimize all the objective functions. However, DAKOTA also identifies a "best" point in the Pareto set defined in terms of distance from the so-called utopia point. The utopia point is defined as the point of extreme best values for each objective. An example from the DAKOTA manual (Adams et al., 2009) highlights this concept. Consider minimizing two objectives simultaneously. If the Pareto front is bounded by (1100) and (90,2), then (1,2) is the utopia point. There will be a point in the Pareto set that has minimum l_2-norm distance to this point. For our problem, each design point corresponds to the fraction of land allocated to Crops 1, 2, and 3. We provide the mean and standard deviation for best solutions from the 240 optimization experiments in Table 3. We also provide the data for the three objective values and the fraction of land allowed to go fallow. Crop 3 has the largest allocation (67%), which is consistent with the fact that it is in the middle in terms of water usage and sales price. Crops 1 and 2 each average around 6% of the land allocation, which is reasonable since there should be some contribution to meeting the demand objective.

Table 2
Model parameters for each crop. Note the relative values between crops for each parameter, giving each an advantage with respect to a distinct objective.

Crop	1	2	3
Yield (Y: Metric Ton/acre)	9.072	2.722	4.536
Sales Price (C_i: \$/Metric Ton)	196.3	604.6	1373.2
Demand (Y_d: Metric Tons)	14,059	4535	9977

Table 3
Mean and standard deviation for the best points (fraction of each crop), function values, and fraction of fallow land obtained from the optimization experiments.

	Mean	Std. dev
Crop 1	0.06	0.03
Crop 2	0.06	0.03
Crop 3	0.67	0.11
Revenue (\$)	14,316,868	3,534,968
Water (m^3)	15,929,621	4,583,874
Demand deviation (Metric Tons)	13,365	1163
Fallow	0.21	0.11

4.3.1. Selected planting scenarios

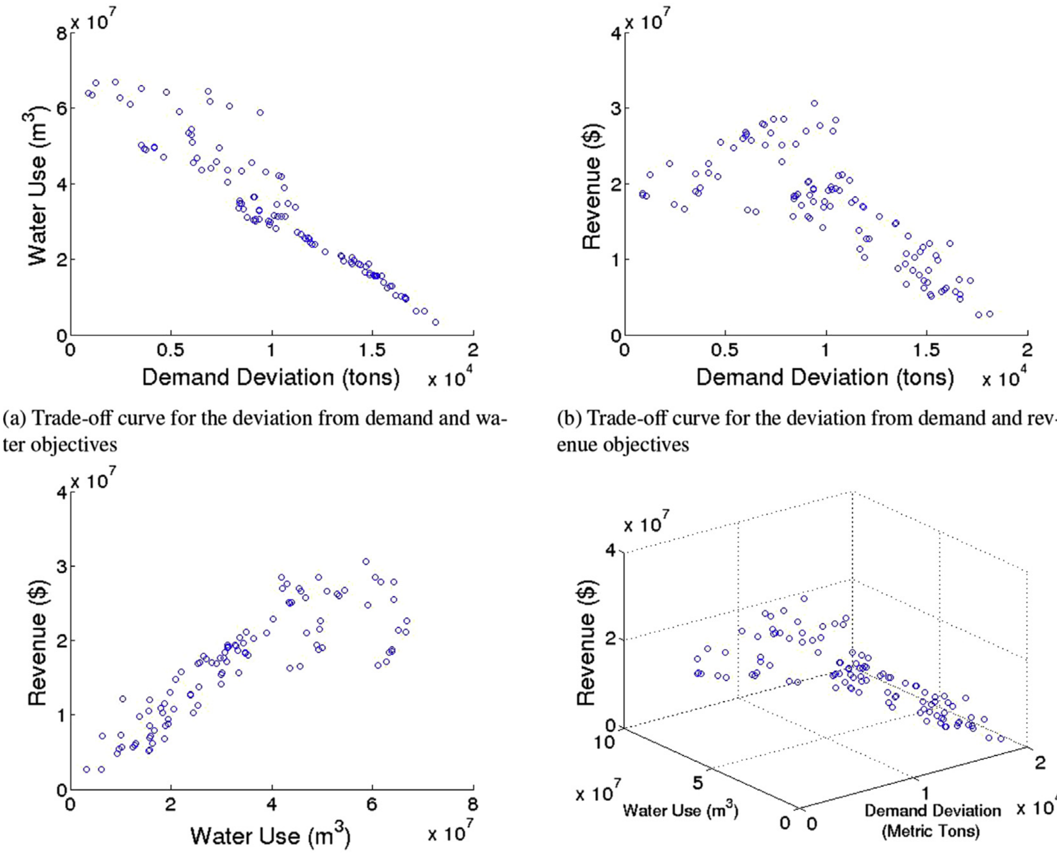
We ran MODFLOW-FMP2 using the crop distributions in Table 3 to illustrate the water usage in relation to the precipitation data incorporated in the model. This is shown in Fig. 4. The behavior shows that during times of insignificant precipitation, pumping is required.

One benefit of obtaining a Pareto set is that stakeholders can select points based on their own criteria. For example, Fig. 5 shows the water usage for one solution with the crop fractions set to (0.40,0.12,0.48) for Crops 1, 2, and 3 respectively. A comparison of the objective values gives a 78% increase in revenue but nearly four times as much water is required. In addition, the new point is 30% closer to meeting the demand. These results highlight how the optimization–simulation approach can provide choices for farmers based on their own priorities.

4.3.2. Optimization performance

For any given optimization experiment we can analyze the trade-off curves between any of the two objectives, which is an inherent strength in using a MOGA in this setting. In fact, these trade-off curves offer alternative solutions to stakeholders based on their own willingness to compromise between competing objectives. We show those in Fig. 6a through c and include a Pareto scatter plot for all three objectives in Fig. 6d. These figures were generated using a population size of 225 and mutation rate of 0.11. The trade-off curves for the revenue and demand objectives (Fig. 6b) and for the water usage and demand objectives (Fig. 6a) show the competing nature of these goals. This also validates that the output from the FMP2 simulations can be used to model the various growing features for the selected crops and provide the appropriate assessments for decision making. In addition, in Fig. 6c the linear dependence of the revenue on the water usage is clear. However, including water usage as a separate objective provides the framework for more sophisticated revenue models that will necessarily incorporate water usage costs. The scatter plot in Fig. 6d shows that the space-filling set of solutions provided by the EA offers farmers a variety of planting options.

One approach to understanding the impact of algorithmic parameters on the final results is to use an analysis of variance (ANOVA) where the algorithm parameters are considered the factors and their different values are taken as the levels. A performance metric is used as the response and the analysis shows whether or not changes in the optimization algorithm parameters have a significant effect on the performance of the algorithm itself. This method can be used to tune optimization algorithms to improve their efficiency for certain classes of problems (Matott et al., 2006). Here we use this approach to understand if changing the population size and mutation rate has a significant impact on the optimization results. We used the hypervolume of the non-



(a) Trade-off curve for the deviation from demand and water objectives

(b) Trade-off curve for the deviation from demand and revenue objectives

(c) Trade-off curve for the water and revenue objectives

(d) Pareto scatter plot for three objectives

Fig. 6. Trade off curves and Pareto scatter plot for three objectives.

dominated space at each generation as a performance metric since DAKOTA uses this metric to guide the optimization. The hypervolume has been shown to be an effective metric in comparing the performance of various EAs and has also been shown to be safer than many other metrics in that it is Pareto-compliant (Fonseca et al., 2005; Zitzler and Thiele, 1999; Minella et al., 2008). Pareto-compliancy indicates that the metric is not susceptible to cases where, when comparing two Pareto front approximations, the front the metric identifies as superior is actually the worse of the two. We use the hypervolume to provide a basis of comparison for the performance of the optimizer given combinations of different population sizes and mutation rates. Since we consider multiple optimization trials, a reference Pareto front was calculated using the combined results of all of our individual optimization runs. An epsilon non-dominated sort is then performed using software produced by Woodruff and Herman (Woodruff and Herman, 2013) and based the algorithm developed by Deb et al. (2005). This returns only those population members which are part of the Pareto front. The hypervolume of the reference Pareto front is then calculated via the same formula used by DAKOTA in its internal calculations (Adams et al., 2009).

$$H = \prod_{j} \mathrm{range(j)}, \tag{6}$$

where H is the hypervolume, j represents a given objective and the range (j) is the difference between the maximum and minimum values of an objective. Finally, we use the hypervolume at the end of each trial and compute a ratio in comparison the reference hypervolume in our ANOVA.

By considering associated p-values, the ANOVA indicated the algorithm parameters had no significant impact on the size of the resulting hypervolumes. The box plots summarizing the data for eight different sets of algorithmic parameters are shown in Fig. 7.

Even though the hypervolume metric is not sensitive to the parameter sets, this doesn't necessarily indicate the algorithm is

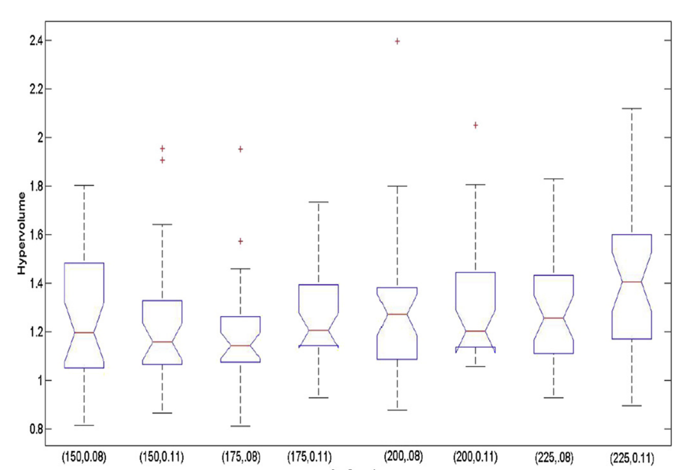


Fig. 7. Box plot of hypervolume data metrics for the different population sizes and mutation rates. Note the insensitivity to changes in algorithmic parameters.

Please cite this article in press as: Fowler, K.R., et al., A decision making framework with MODFLOW-FMP2 via optimization: Determining trade-offs in crop selection, Environmental Modelling & Software (2014), http://dx.doi.org/10.1016/j.envsoft.2014.11.031

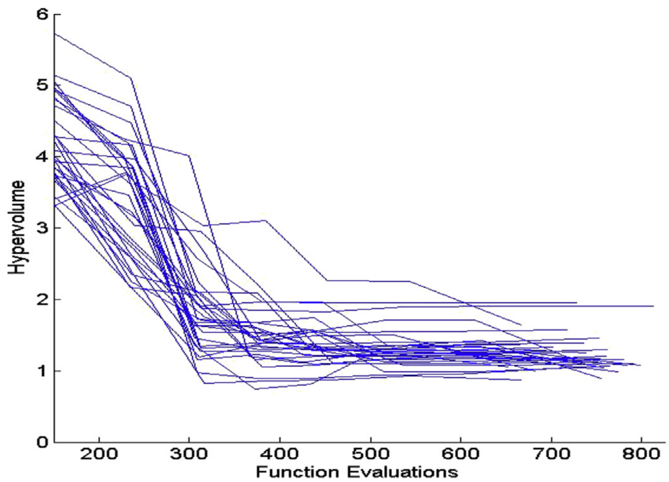


Fig. 8. Iteration history for 30 optimization trials with a population size of 175 and mutation rate of 0.11 showing primarily insignificant changes in the hypervolume size after a sufficient number of function evaluations.

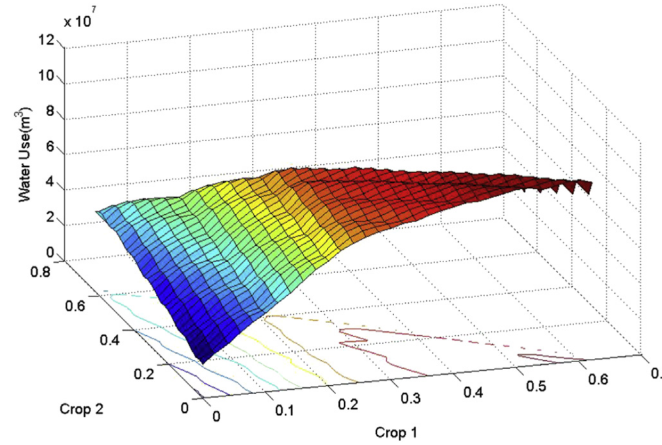


Fig. 10. Water usage landscape for Crops 1 and 2 while Crop 3 is fixed at 0.36.

performing well. To better understand the iteration history, we consider the size of the hypervolumes as the optimization progresses. Fig. 8 shows the hypervolume sizes as the number of function evaluations increases, generated using the output from the 30 trials with a population size of 175 and a mutation rate of 0.11. Multiple plots of this type were generated and all showed similar behavior. The size of the hypervolumes shows no significant change long before the function evaluation budget is exceeded, indicating a higher budget would not necessarily improve the results.

4.4. Optimization landscapes

For this problem, it is straightforward to generate optimization landscapes by fixing one crop distribution and letting the other two vary over the feasible region while evaluating the demand, water usage, and profit objectives. These are shown in Figs. 9 through 11c. Specifically, the landscapes were generated by fixing one crop then varying the other two by increments of 0.02. The crop fractions for these figures were set to Crop 1 fixed at 0.25, Crop 2 at 0.27, and Crop 3 at 0.36. These values were chosen to capture a snapshot of each crops properties (in terms of profitability, water use, and demand) on those competing objectives. These assignments allow the other two crops to vary over a wide range of values as an attempt to illustrate features of the landscapes. For example, a value of crop 3 at 0.36 means the for all other combinations of crops 1 and 2, crop 3 will still be the highest, which highlights the fact that crop 3 has the highest demand. Since the decision variables are the fractions of crops allocated to the farm and this fraction is then implemented in the FMP2 framework, the accuracy is limited to 0.001. For example, if the optimizer suggested 0.322 as a fraction for Crop 1, this would be implemented as 0.32 in our 100 cell example. This generated a total of nine landscapes, and we show a representative subset here.

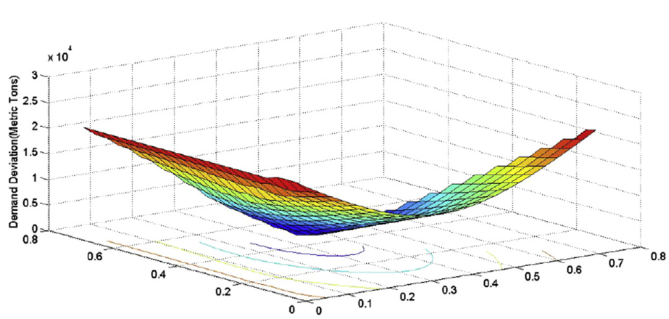


Fig. 9. Demand landscape for Crops 1 and 3 while Crop 2 is fixed at 0.27. Note the quadratic surface.

Since the deviation from demand is modeled using the l_2 norm, the landscapes in which a crop is fixed are naturally quadratic, as seen in Fig. 9. The other two demand landscapes looked similar.

Recall that the water usage for Crop 1 was the highest, Crop 2 was the lowest, and Crop 3 was in the middle. We show the corresponding surface for Crop 3 fixed in Fig. 10. The result shows small plateaus in the optimization landscapes and large regions with minimal changes in water usage. These properties create local minima that can trap gradient based methods or stencil based methods when a sufficiently small increment is used (Fowler et al., 2004, 2008). Fig. 10 demonstrates the output from physically-based, multi-model simulators can result in challenging landscapes for classic optimization approaches. This supports the choice of an EA, which doesn't require gradients, and has strong global search properties to avoid local minima.

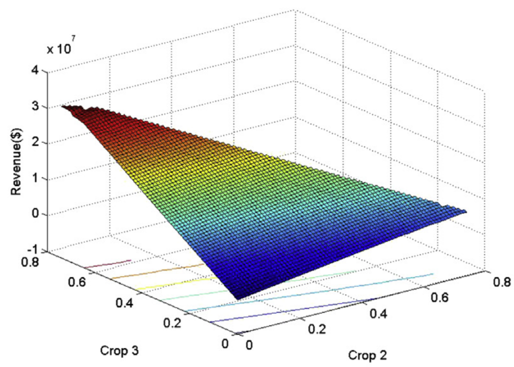
We show all three scenarios for the revenue landscapes in Fig. 11a through c. Overall, these landscapes demonstrate the impact of heavily water-dependent crops on revenue. In Fig. 11a, Crop 1, which is the most water-intensive crop with the largest sales price, is fixed. The landscape shows linear dependence of revenue on the other two crops. However, once Crop 1 is allowed to vary, as in Fig. 11b–c, the landscapes are no longer uniformly linear.

Specifically, observe that for roughly 20% of Crop 1 and 53% of Crop 3, there is a distinct maximum revenue as shown in Fig. 11b. Note that while it appears from a brief glance that Crop 3 produces the greatest revenue per acre, crops such as alfalfa are able to produce multiple yields per growing season. This in addition to the nonlinearity in our revenue objective introduced by inclusion of water costs adds complexity to what would otherwise be a simple outcome for our revenue results.

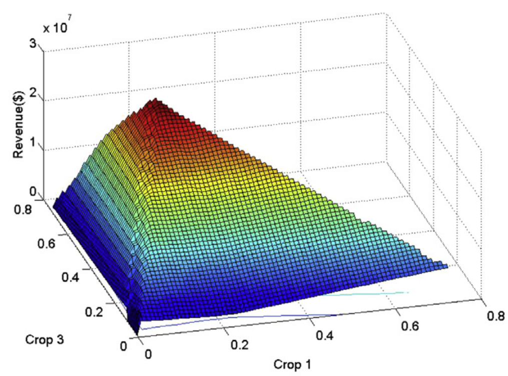
In Fig. 11c, Crop 3 is fixed. The landscape shows that after roughly 20% of Crop 1 is planted, the revenue landscape plateaus. Given a limit on groundwater extractions, planting too much of Crop 1 could lead to a deficit irrigation situation. In a deficit situation yield is affected thereby leading to a decrease in revenue.

5. Conclusions and future work

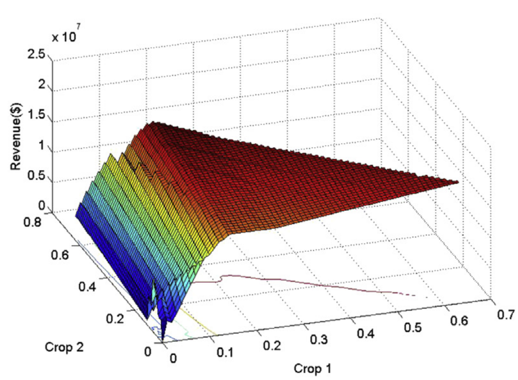
This was a first effort to exploit the sophisticated interactions of the agricultural-ground water flow model MODFLOW-FMP2 within



(a) Revenue landscape for Crops 2 and 3 while Crop 1 is fixed at 0.25.



(b) Revenue landscape for Crops 1 and 3 while Crop 2 is fixed at 0.27.



(c) Revenue landscape for Crops 1 and 2 while Crop 3 is fixed at0.36.

Fig. 11. Revenue landscapes.

an optimization framework. This work facilitates future studies which will assess the impact of farm-scale or regional scale agricultural practices on underlying aquifers by moving beyond the simple comparisons from running different model scenarios. Our approach shows that MODFLOW-FMP2 can be used in a simulation-based design framework to allow for flexibility in choosing optimization tools, analyzing the impacts of model parameters on farming decisions, and considering a broad range of critical objective functions. The multi-objective evolutionary algorithm (MOGA) chosen from the DAKOTA optimization package provided promising results on the three competing objectives. The DAKOTA software tool offers a suite of optimization options; we chose MOGA since as, an evolutionary algorithm, it naturally has strong space-filling and global search capabilities. The use of MOGA within DAKOTA also directly facilitates the analysis of trade-off curves and provides performance metrics. Future work will include a comparison of optimization approaches as well as modeling scenarios to better understand performance interactions and provide further guidance in choosing optimization strategies.

There are, however, a number of directions for advancing this research. In particular, a next step is to allow for dynamic planting decisions so that when a crop is harvested, the optimizer may act as a dynamic virtual farmer to select from the feasible set of crops available for planting. This more realistic scenario requires additional constraints to manage the growing and harvesting schedules of crops (Bokhiria et al., 2014). In addition, the time horizons need to be extended to allow for increased variation of water prices, sales prices, labor fixed costs, market demands, and other factors not considered in the revenue and profit models used here.

Additional constraints enforcing the maximum 20% fluctuations in crop portfolios or other common farming practices could be included, but focused collaborations between the farming and scientific communities are needed to better understand the dynamics behind the farming realities. Moreover, imposing a wider range of hydrological or conjunctive use constraints, e.g., limiting values of hydraulic head at pumping wells near critical features of the domain, should be enforced to better understand the underlying models. Previous work (Fowler et al., 2004, 2008) highlighted the influence these types of constraints have on optimization landscapes, leading to non-convexities and discontinuous feasible regions and further supporting the use of evolutionary algorithms as a global search tool.

Perhaps the greatest opportunity for extensions of this work is in the development and testing of relevant objective functions to represent the interest of stakeholders in a given region. An advantage of this simulation–optimization framework is that essentially any input and output from the simulator can be used to guide decision makers. A user is free to design any objective representing their own interest given that MODFLOW-FMP2 can provide the relevant output for a function evaluation. This work is only a starting point for understanding how one might take advantage of the detailed, predictive capabilities of that software. For example, although the types of crops in this problem were fixed, an alternate formulation may allow the optimizer to determine crop model parameters leading to sustainable water usage. In that case, solutions would provide lists of the types of crops ideal for a given region and climate. In addition, the focus of this work was on reducing groundwater pumping through crop selection. MODFLOW-FMP2 incorporates multiple irrigation strategies that can also be considered in other management objectives. Future work will incorporate the recently released MODFLOW-OWHM simulation tool (Hanson et al., 2014a), a modification of MODFLOW-FMP2 which includes, in part, better metrics for water tracking and an enhancement of conjunctive use models.

Sensitivity analyses are recommended with the development of new objectives to understand the impact of physical model parameters on problem solutions, as well as the impact of numerical parameter settings (such as grid resolution or internal solver tolerances, see Farthing et al. (2012)) and optimization algorithmic parameter settings. In this work, we used an ANOVA approach to show that for our three objectives, results were not sensitive to the population size and mutation rate. As pointed out in the work by Maier et al. (2014), understanding the fundamental algorithm search behavior and algorithm performance assessments are ongoing research challenges when applying metaheuristics to water resource problems.

Since the simulation-model is decoupled from the optimizer, only the management of input and output is required. We should note that manipulating the data files for MODFLOW-FMP2 requires knowledge of the underlying models and can take effort to implement. The open-source GUI Model Viewer, also developed by the USGS, is a helpful tool in creating the necessary hydrological models underlying the farm process models used by MODFLOW-FMP2 (Sieh and Winston, 2002). The MODFLOW-FMP2 software package provides several examples to facilitate the creation of farm models as well as a database with over 450 crop parameters (Schmid and Hanson, 2009).

To promote the use of the simulation–optimization framework presented here, the hydrological data files for the example problem presented in this paper as well as the python wrappers and objective functions are provided online at http://people.clarkson.edu/kfowler/Sustainability.html. The required links to compile DAKOTA and MODFLOW-FMP2 are provided.

Acknowledgments

The authors wish to thank Dr. Randall Hanson of the United States Geological Survey for his assistance in coupling external software with the MODFLOW-FMP2 simulation tool, as well as the many useful discussions and insights on various aspects of the simulation tool. We also thank Dr. Stacy Howington of ERDC USACE for guidance on the hydrology. We also thank Stephen Carter of Mathworks for his initial algorithm development. This work was supported in part through an American Institute of Mathematics SQuaRE grant.

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Please cite this article in press as: Fowler, K.R., et al., A decision making framework with MODFLOW-FMP2 via optimization: Determining trade-offs in crop selection, Environmental Modelling & Software (2014), http://dx.doi.org/10.1016/j.envsoft.2014.11.031